Mimetic Finite Difference Methods on Unstructured Polyhedral Meshes

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National Nuclear Security Administration

MICS Mathematical, Information, and Computational Sciences

ASC

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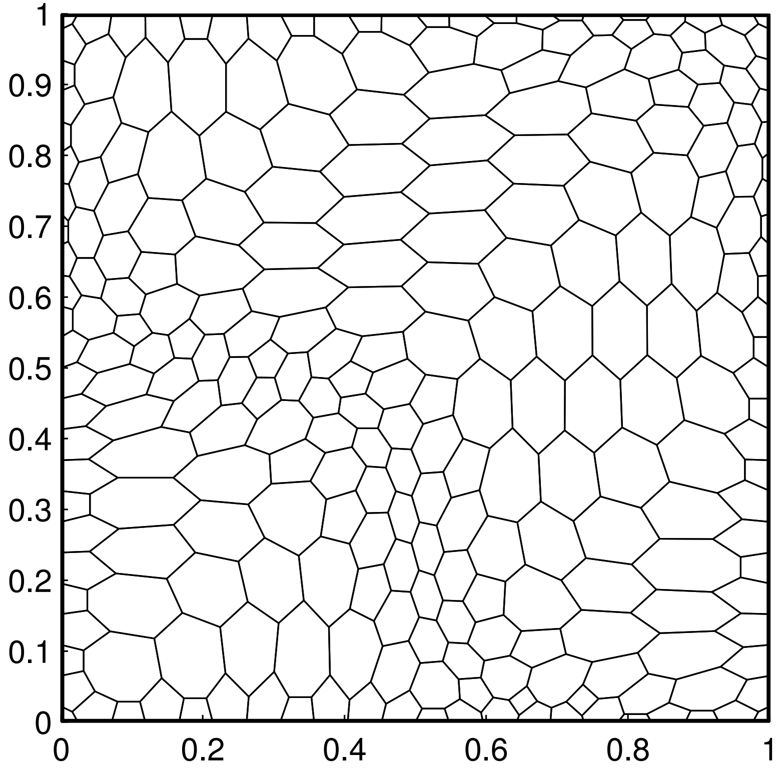
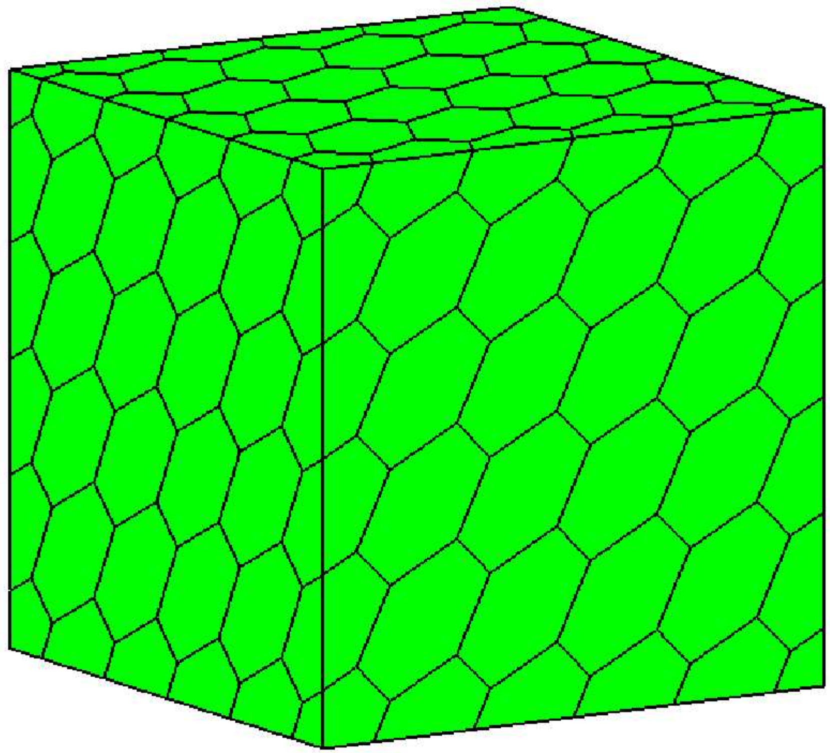
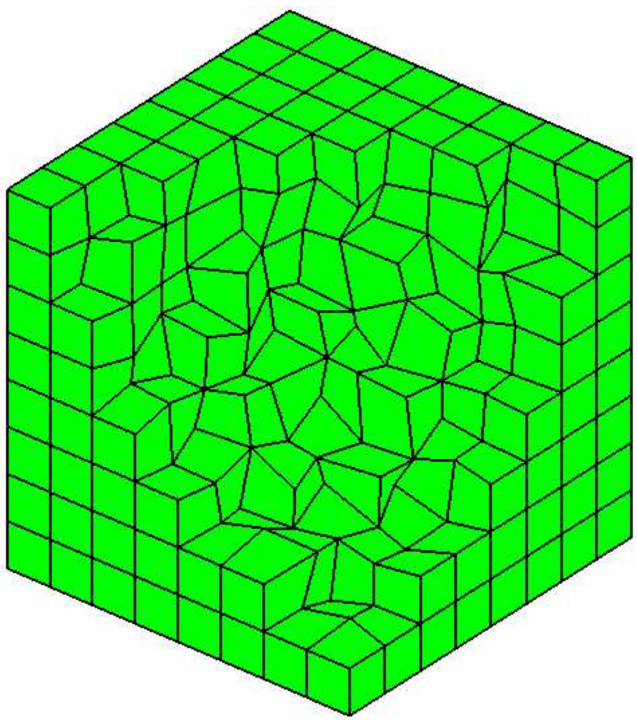
Problem formulation

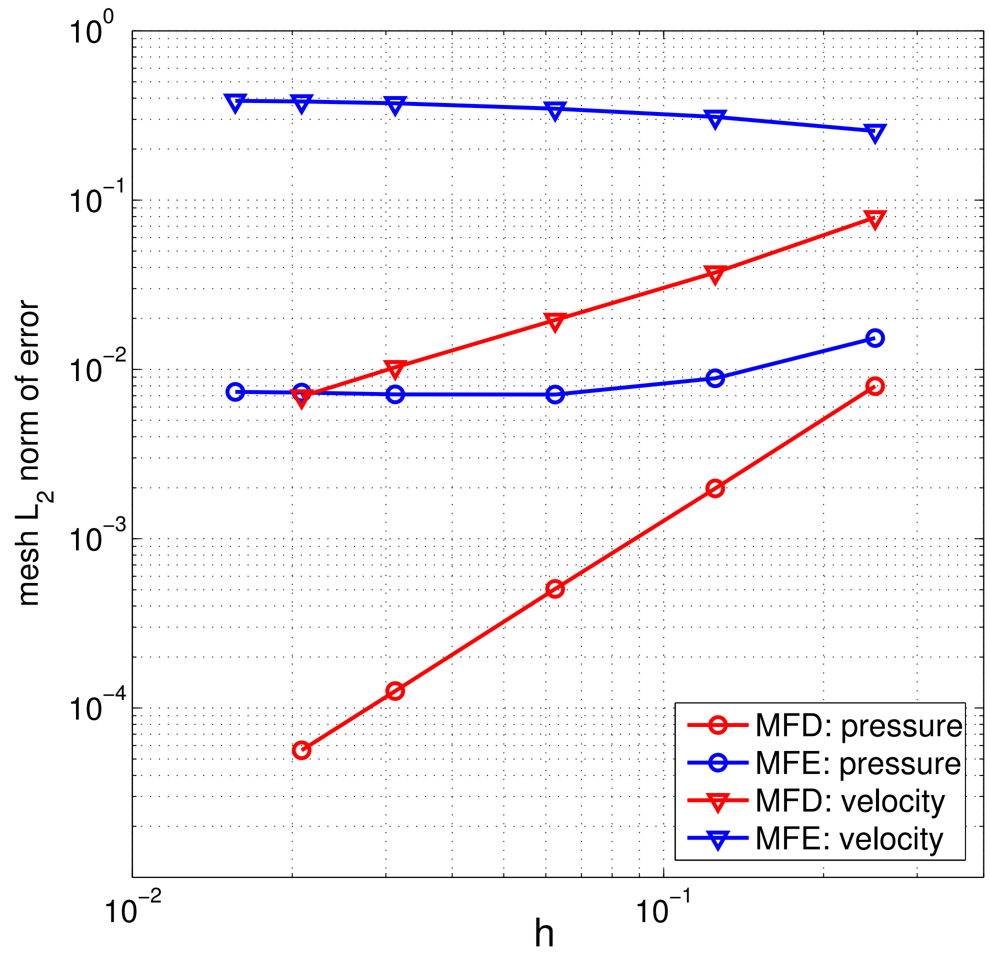




- polyhedral meshes are preferable for some CFD applications
- moving mesh methods (Lagrangian, ALE) result in non-planar faces
- unlimited possibilities for mesh generation

Problem formulation (cont.)





- the mixed FE method does *not* converge on randomly perturbed meshes

Mimetic finite difference method

Continuum Problem	MFD method
$$\begin{aligned} \mathrm{div}\vec{u} &= b \\ \vec{u} &= -\nabla p \end{aligned}$$	$$\begin{aligned} \mathcal{DIV}\boldsymbol{u}^h &= \boldsymbol{b}^h \\ \boldsymbol{u}^h &= -\mathcal{GRAD}\boldsymbol{p}^h \end{aligned}$$
■ $\mathrm{div} = -\nabla^*$ ■ $\ker(\nabla) = constants$	■ $\mathcal{DIV} = -\mathcal{GRAD}^*$ ■ $\ker(\mathcal{GRAD}) = constants$

Mimetic finite difference method

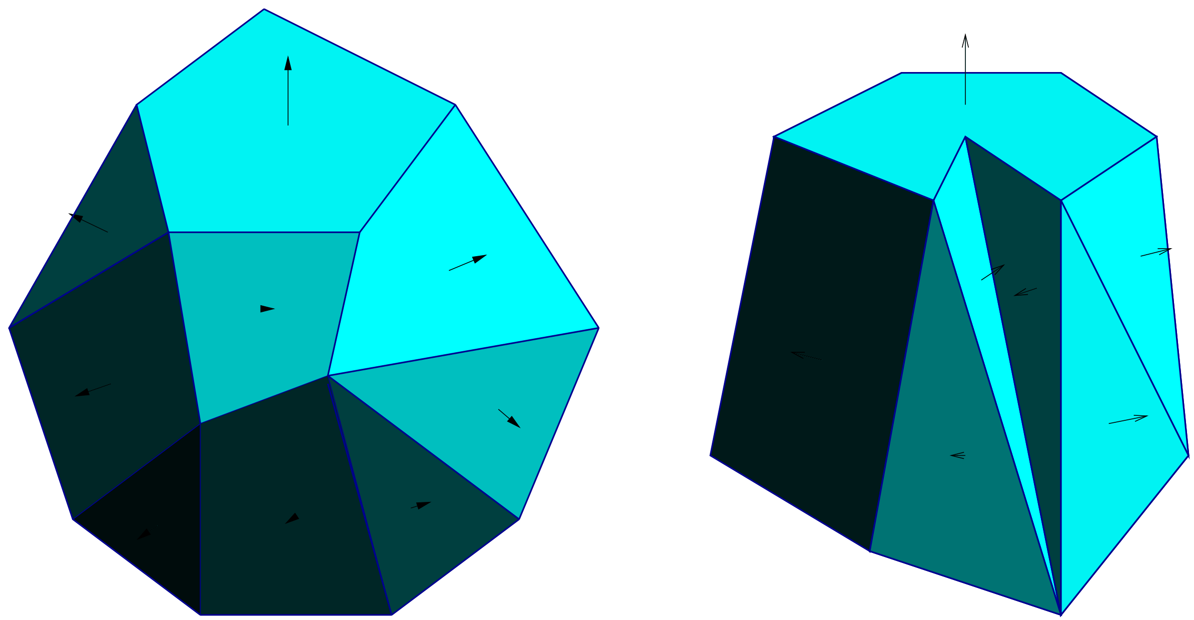
$$\nabla = -\mathrm{div}^* \qquad\qquad \ker(\nabla) = constants$$

Four-step methodology:

1. Define degrees of freedom for $\boldsymbol{p}^h \in Q_h$ and $\boldsymbol{u}^h \in X_h$
2. Discretize the divergence operator, $\mathcal{DIV}$
3. Equip discrete spaces with inner products $[\cdot\,,\,\cdot]_Q$ and $[\cdot\,,\,\cdot]_X$
4. Derive the gradient operator, $\mathcal{GRAD}$, from discrete Green's formula

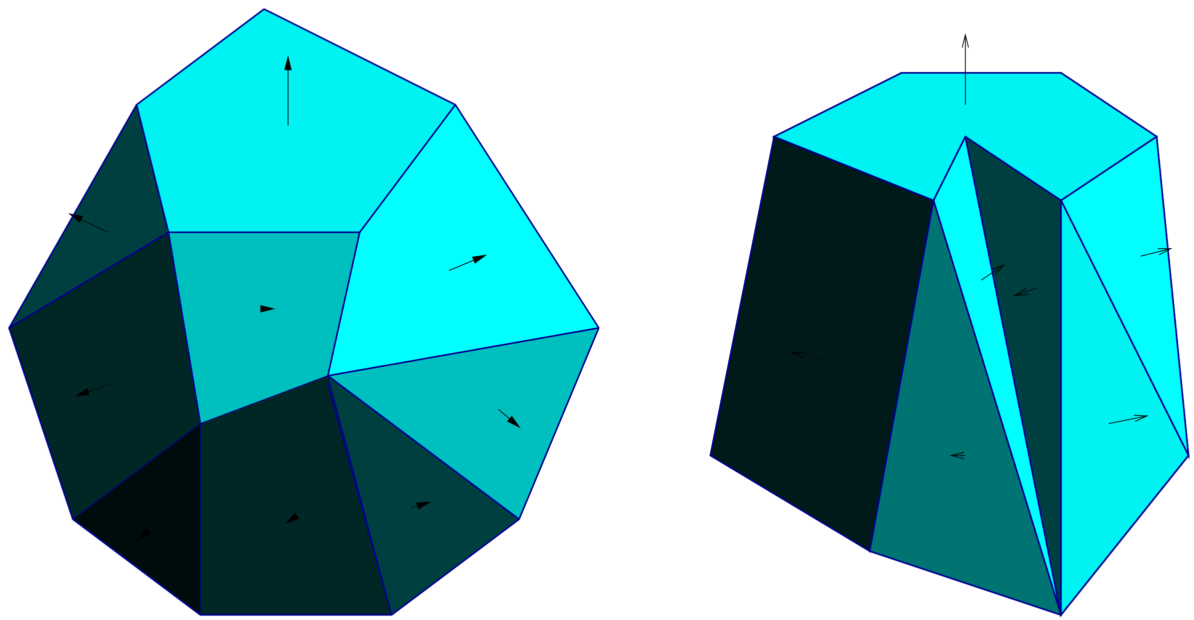
$$\mathcal{GRAD} = -\mathcal{DIV}^* \qquad\qquad \ker(\mathcal{GRAD}) = constants$$

Degrees of freedom for p^h and u^h



- $\boldsymbol{p}^h$ is constant on E
  - p_E^h is the degree of freedom associated with element E

Degrees of freedom for p^h and u^h

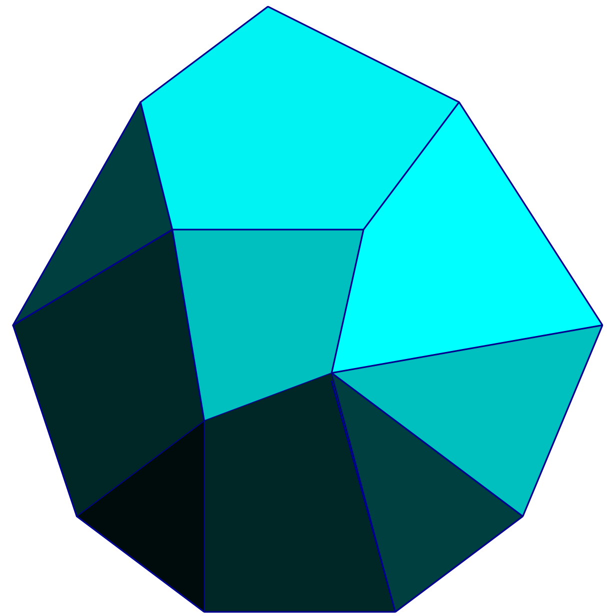


- $\boldsymbol{u}^h$ is constant on faces of E
  - u_f^h is the normal velocity component associated with face f

Divergence operator

Divergence theorem:

$$\int_E \operatorname{div} \vec{u} = \oint_{\partial E} \vec{u} \cdot \vec{n}$$



implies

$$\left(\mathcal{DIV}\, \boldsymbol{u}^h\right)_E = \frac{1}{|E|} \sum_{f \in \partial E} u_f^h \, |f|$$

Inner products

- $$[\boldsymbol{p}^h,\, \boldsymbol{q}^h]_Q = \sum_{E\in\Omega_h} p_E^h\, q_E^h\, |E|$$

- $$[\boldsymbol{u}^h,\, \boldsymbol{v}^h]_X = \sum_{E\in\Omega_h} [\boldsymbol{u}^h,\, \boldsymbol{v}^h]_E$$

$$[\boldsymbol{u}^h,\, \boldsymbol{v}^h]_E = \sum_{i,j=1}^{k_E} \mathbb{M}_{E,i,j}\, u_{f_i}^h\, v_{f_j}^h$$

where $\mathbb{M}_E = {\mathbb{M}_E}^T > 0$ and k_E is the number of faces of E.

Gradient operator

- The Green formula

$$\int_\Omega \vec{u} \cdot \nabla p = -\int_\Omega p \operatorname{div} \vec{u}.$$

- The discrete Green formula

$$[\boldsymbol{u}^h, \mathcal{GRAD}\, \boldsymbol{p}^h]_X = -[\boldsymbol{p}^h, \mathcal{DIV}\, \boldsymbol{u}^h]_Q$$

defines the gradient operator.

Properties of the discretization

- solution algorithm results in a problem with the SPD matrix
- full diffusion tensor is easily incorporated into the discretization methodology
- 2nd order accurate for pressure variable when elements have planar (or slightly perturbed) faces
- 1st order accurate for velocity variable

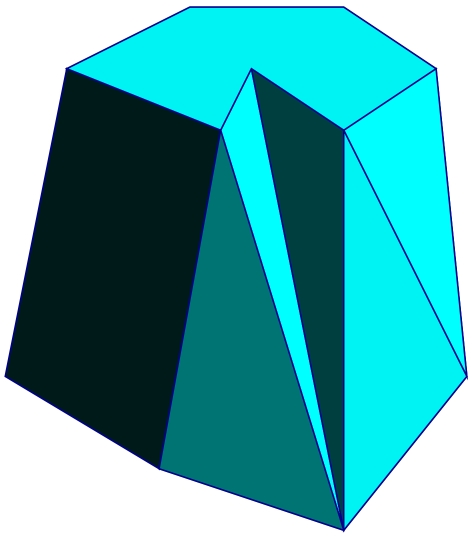
Convergence analysis

Our theory forbids:

- anisotropic (stretched) elements
- stretched faces
- small 2D angles

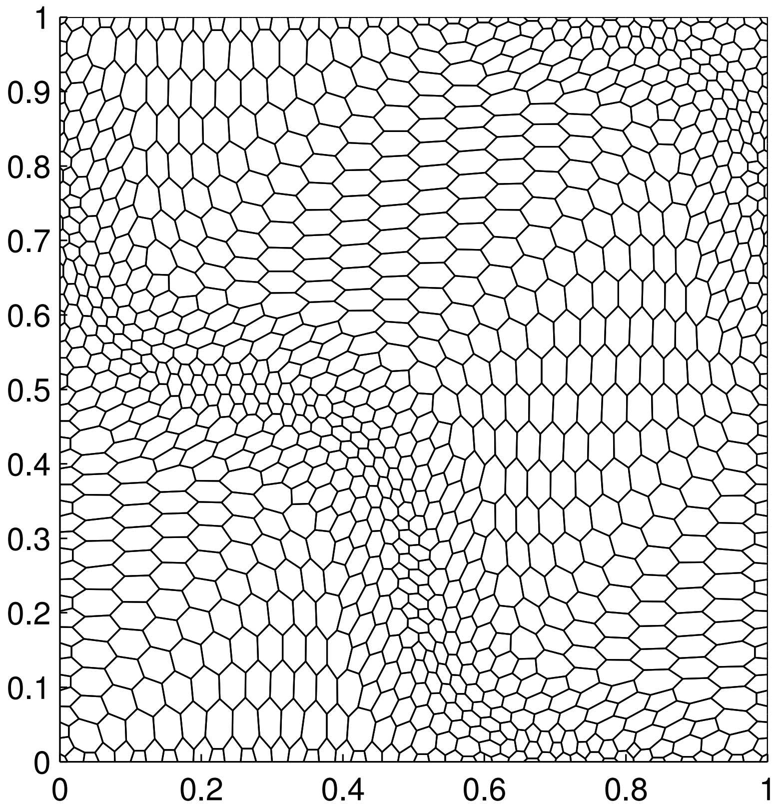
Our theory allows:

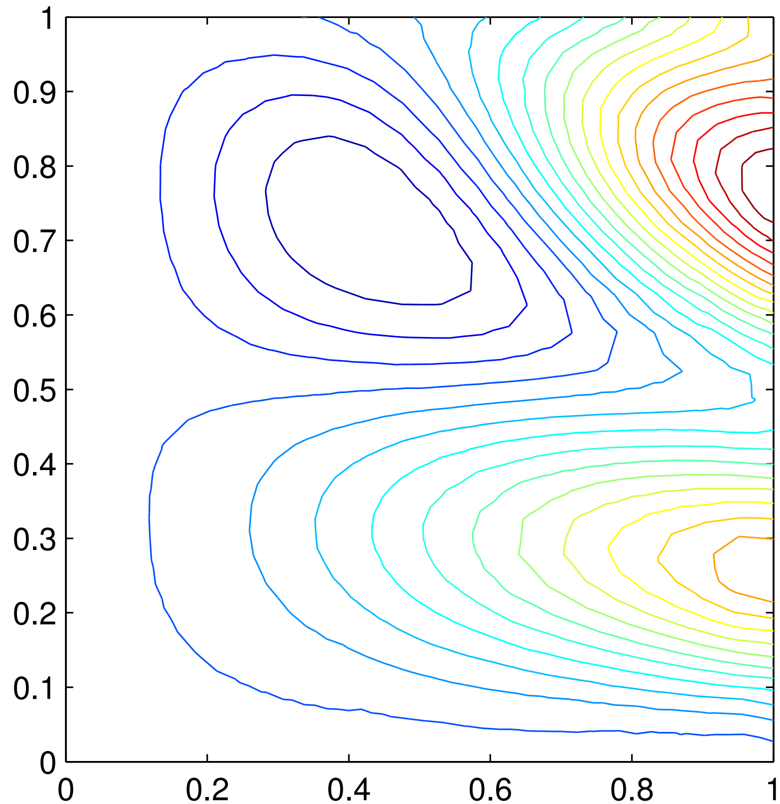
- regular meshes
- degenerate elements
- non-convex elements



Polygonal meshes

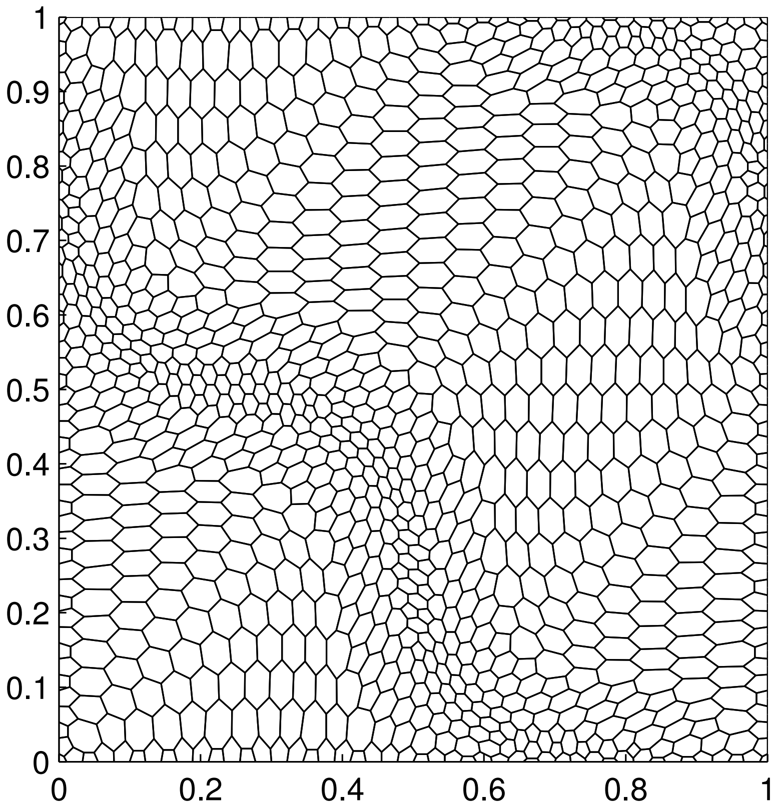
$$p(x,\,y) = x^3y^2 + x\sin(2\pi xy)\sin(2\pi y), \qquad \mathbb{K} = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}$$

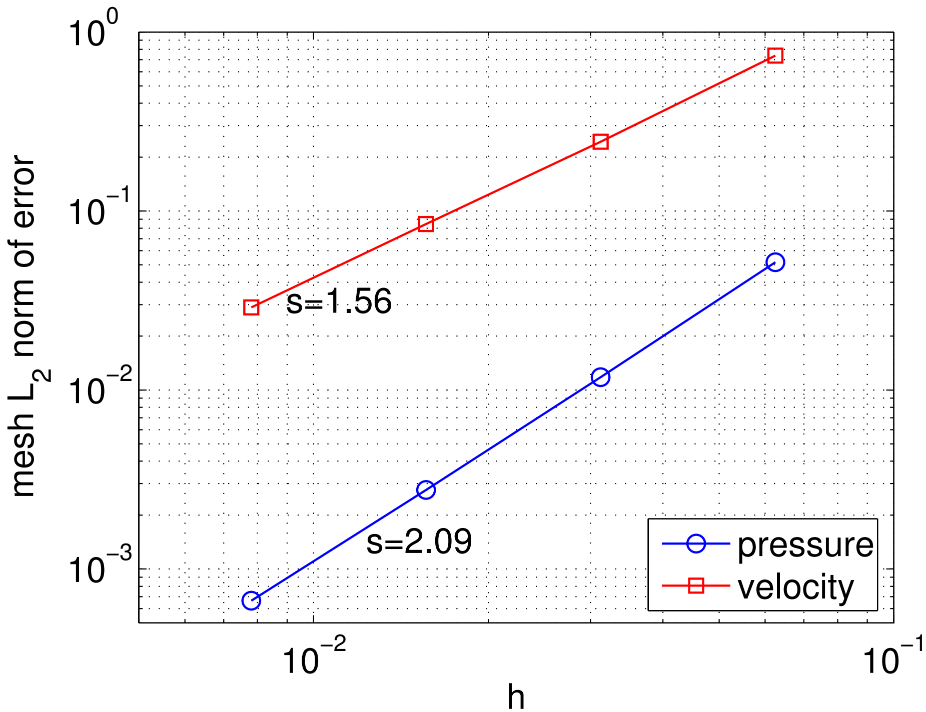




Polygonal meshes

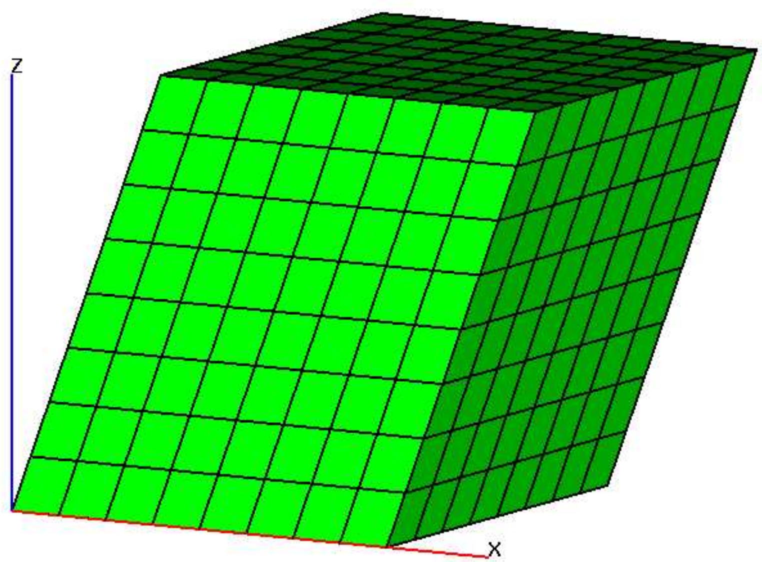
$$p(x,\, y) = x^3y^2 + x\sin(2\pi xy)\sin(2\pi y), \qquad \mathbb{K} = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}$$

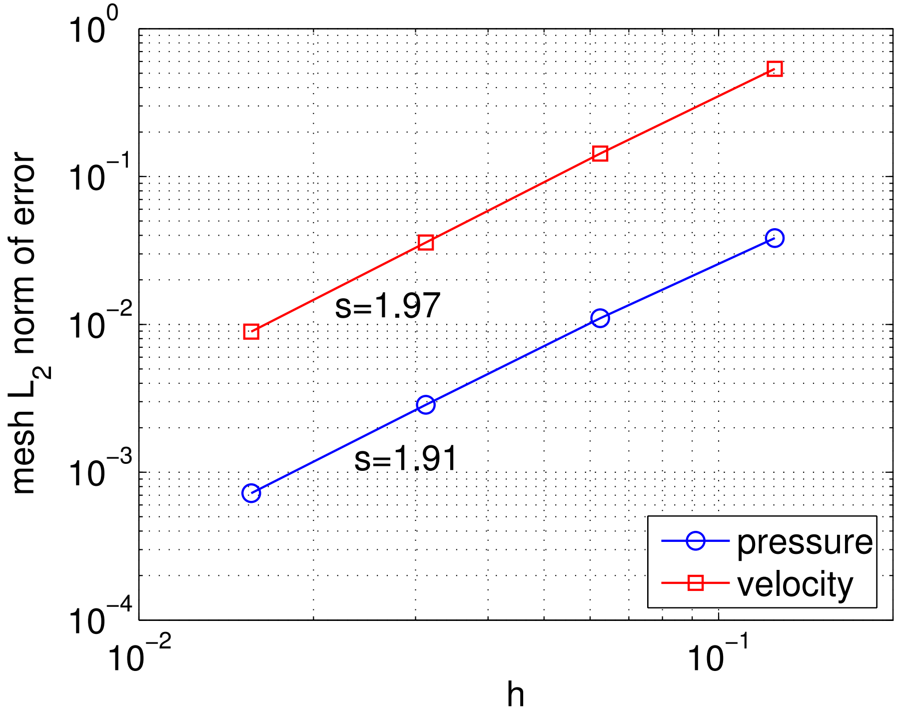




Polyhedral meshes

Problem similar to the above 2D problem





Key element of the MFD method

$$\boxed{[\boldsymbol{u}^h,\, \boldsymbol{v}^h]_E = \sum_{i,j=1}^{k_E} \mathbb{M}_{E,i,j}\, u^h_{f_i}\, v^h_{f_j}}$$

- Condition I: spectrally equivalent to a diagonal matrix:

$$\mathbb{M}_E \sim \begin{pmatrix} |E| & & \\ & \ddots & \\ & & |E| \end{pmatrix}$$

- Condition II: exact for linear pressure p^1 ($\vec{u}^1 = \nabla p^1 = const$):

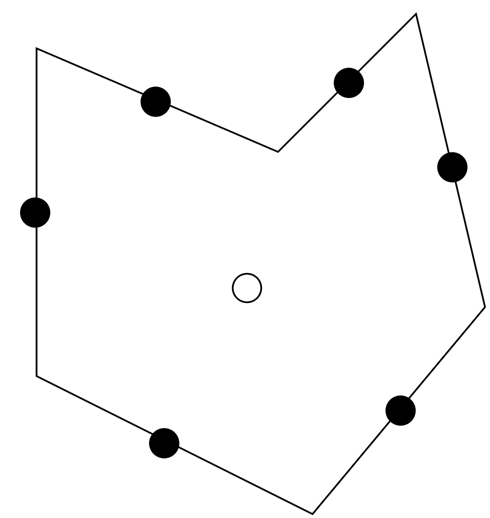
$$[(\nabla p^1)^h,\, \boldsymbol{v}^h]_E \equiv -\int_E p^1 (\mathcal{DIV}\boldsymbol{v}^h)_E + \sum_{f\in\partial E} v^h_f \int_f p^1$$

Key element of the MFD method

$$\boxed{[\boldsymbol{u}^h,\ \boldsymbol{v}^h]_E = \sum_{i,j=1}^{k_E} \mathbb{M}_{E,i,j}\, u^h_{f_i}\, v^h_{f_j}}$$

- Condition II: exact for linear pressure p^1 ($\vec{u}^1 = \nabla p^1 = const$):

$$\begin{bmatrix} \vec{u}^1 \cdot \vec{n}_1 \\ \vec{u}^1 \cdot \vec{n}_2 \\ \vdots \\ \vec{u}^1 \cdot \vec{n}_6 \end{bmatrix} = \mathbb{M}_E^{-1} \begin{bmatrix} |f_1|\,(p^1(\boldsymbol{x}_1) - p^1(\boldsymbol{x}_0)) \\ |f_2|\,(p^1(\boldsymbol{x}_2) - p^1(\boldsymbol{x}_0)) \\ \vdots \\ |f_6|\,(p^1(\boldsymbol{x}_6) - p^1(\boldsymbol{x}_0)) \end{bmatrix}$$

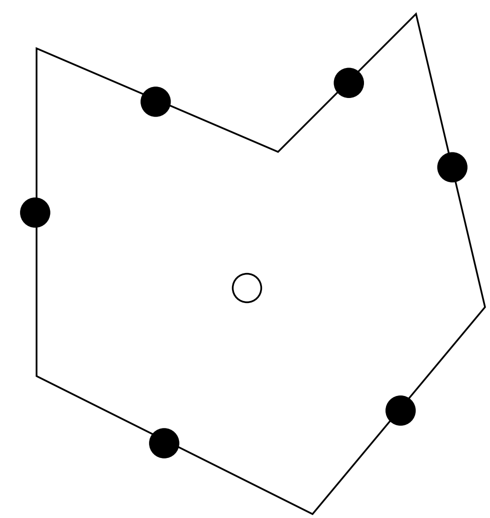


Key element of the MFD method

$$\boxed{[\boldsymbol{u}^h,\ \boldsymbol{v}^h]_E = \sum_{i,j=1}^{k_E} \mathbb{M}_{E,i,j}\, u^h_{f_i}\, v^h_{f_j}}$$

- Condition II: take $p^1 = x$, then $\vec{u} = (1,\ 0)^T$ and

$$\begin{bmatrix} n_{1,x} \\ n_{2,x} \\ \vdots \\ n_{6,x} \end{bmatrix} = \mathbb{M}_E^{-1} \begin{bmatrix} |f_1|\,(x_1 - x_0) \\ |f_2|\,(x_2 - x_0) \\ \vdots \\ |f_6|\,(x_6 - x_0) \end{bmatrix}$$



Key element of the MFD method

$$\left[\boldsymbol{u}^h,\ \boldsymbol{v}^h\right]_E = \sum_{i,j=1}^{k_E} \mathbb{M}_{E,i,j}\, u^h_{f_i}\, v^h_{f_j}$$

- Condition II: take $p^1 = y$, then $\vec{u} = (0,\ 1)^T$ and

$$\begin{bmatrix} n_{1,x} & n_{1,y} \\ n_{2,x} & n_{2,y} \\ \vdots & \\ n_{6,x} & n_{6,y} \end{bmatrix} = \mathbb{M}_E^{-1} \begin{bmatrix} |f_1|\,(x_1 - x_0) & |f_1|\,(y_1 - y_0) \\ |f_2|\,(x_2 - x_0) & |f_1|\,(y_2 - y_0) \\ \vdots & \vdots \\ |f_6|\,(x_6 - x_0) & |f_1|\,(y_6 - y_0) \end{bmatrix}$$

$$\mathbb{N}_{6\times 2} = \mathbb{M}_E^{-1}\, \mathbb{R}_{6\times 2}$$

Properties of matrices $\mathbb{N}$ and $\mathbb{R}$

Lemma.

$$\mathbb{N}^T \mathbb{R} = \mathbb{R}^T \mathbb{N} = \mathbb{I}_{2\times 2}$$

Proof.

$$\begin{aligned}
|E| = \int_E \nabla x \cdot \nabla (x - x_0) &= \int_{\partial E} (\nabla x \cdot \vec{n})(x - x_0) = \sum_i n_{i,x} \int_{e_i} (x - x_0) \\
&= \sum_i n_{i,x} |e_i| (x_i - x_0) = \sum_i \mathbb{N}_{i,1} \mathbb{R}_{i,1} \\
&= (\mathbb{N}^T \mathbb{R})_{1,1}
\end{aligned}$$

Similarly,

$$0 = \int_E \nabla y \cdot \nabla (x - x_0) = \int_{\partial E} (\nabla y \cdot \vec{n})(x - x_0) = (\mathbb{N}^T \mathbb{R})_{2,1}$$

Simple formula for $\mathbb{M}_E^{-1}$

A solution to

$$\mathbb{N} = \mathbb{M}_E^{-1}\,\mathbb{R} \equiv \mathbb{W}\,\mathbb{R}$$

is

$$\mathbb{W}_0 = \mathbb{N}\,\mathbb{N}^T$$

- check: $\mathbb{W}_0\,\mathbb{R} = \mathbb{N}\,\mathbb{N}^T\,\mathbb{R} = \mathbb{N}\,\mathbb{I} = \mathbb{N}$
- valid for *any* polygon and *any* polyhedron with planar faces
- $\mathbb{W}_0 = \mathbb{W}_0^T \geq 0$
- general form for the solution is $\mathbb{W}_0 + \mathbb{W}_1$ where $\mathbb{W}_1\,\mathbb{R} = 0$

Simple formula for $\mathbb{M}_E^{-1}$ (cont.)

Theorem. Let columns of $\mathbb{D}$ span $\ker(\mathbb{R}^T)$, i.e.

$$\mathbb{R}^T\,\mathbb{D} = 0 \qquad \text{and} \qquad \mathbb{D}^T\,\mathbb{R} = 0.$$

Then,

$$\mathbb{M}_E^{-1} = \mathbb{N}\,\mathbb{N}^T + \mathbb{D}\,\mathbb{U}\,\mathbb{D}^T$$

is the SPD matrix for any $\mathbb{U} = \mathbb{U}^T > 0$.

Simple formula for $\mathbb{M}_E^{-1}$ (cont.)

$$\mathbb{M}_E^{-1} = \mathbb{N}\,\mathbb{N}^T + \mathbb{D}\,\mathbb{U}\,\mathbb{D}^T$$

Let $\tilde{\mathbb{D}}$ be symmetric orthogonal projector onto $\ker(\mathbb{R}^T)$ and

$$\mathbb{U} = u\mathbb{I}, \qquad u = \frac{1}{|E|}.$$

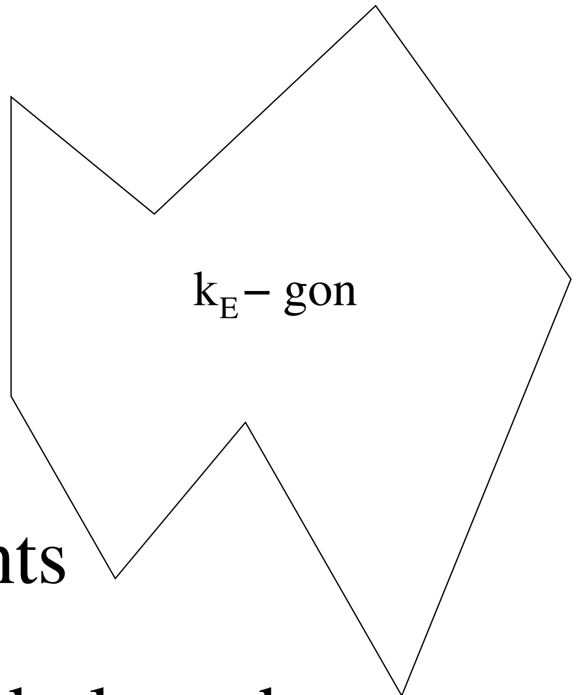
Then

$$\boxed{\mathbb{M}_E^{-1} = \mathbb{N}\,\mathbb{N}^T + u\tilde{\mathbb{D}}}$$

- computing of $\mathbb{M}_E^{-1}$ requires $(2d+1)k_E^2 + 4d^2 k_E$

Family of MFD methods

$$\mathbb{M}_E^{-1} = \mathbb{N}\,\mathbb{N}^T + \mathbb{D}\,\mathbb{U}\,\mathbb{D}^T$$

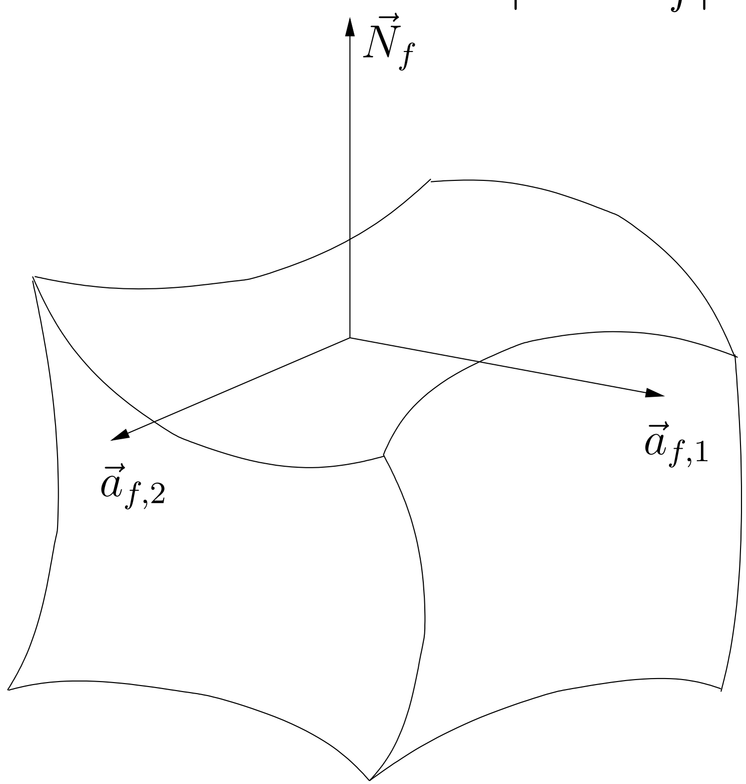


- size of $\mathbb{U}$ is $k_E - 2$
- $(k_E - 1)(k_E - 2)/2$ free coefficients
- the same formula holds for polyhedral meshes
- straightforward generalization to full material tensor

Strongly curved faces

- the mesh face f is called *strongly curved* if

$$|\vec{n} - \vec{N}_f| > \sigma |f|^{1/2} \qquad \vec{N}_f = \frac{1}{|f|}\int_f \vec{n}.$$



- 3 d.o.f. (3 components of a velocity vector) per *strongly curved* mesh face

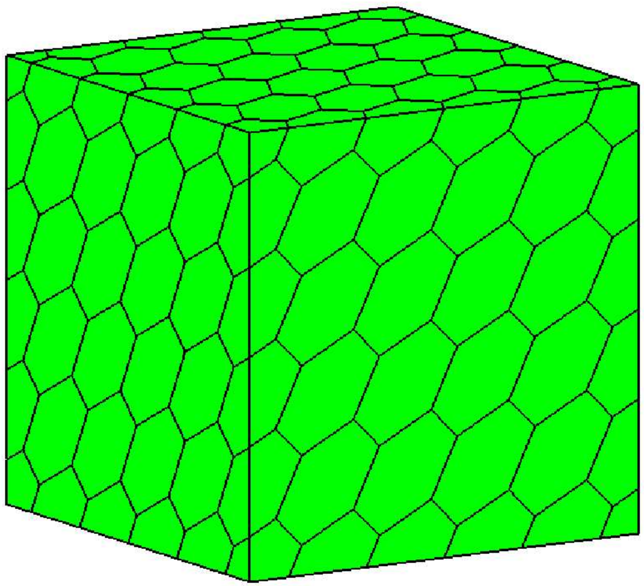
$$\boldsymbol{u}_f^h \cdot \vec{N}_f = \frac{1}{|f|}\int_f \vec{u}\cdot\vec{n}$$

and

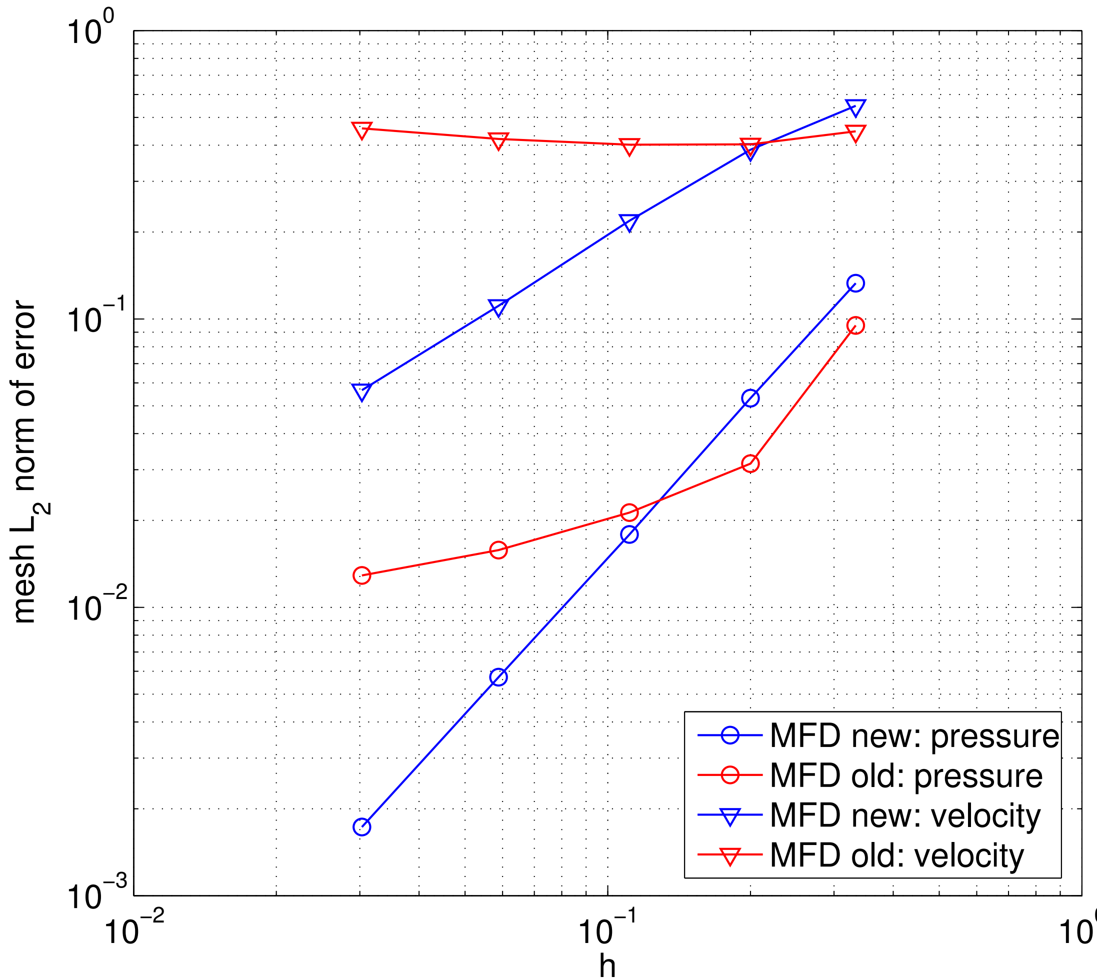
$$\boldsymbol{u}_f^h \cdot \vec{a}_{f,i} = \frac{1}{|f|}\int_f \vec{u}\cdot\vec{a}_{f,i} \quad i = 1, 2.$$

- the matrix $\mathbb{M}_E^{-1}$ is generated as it was described above!

Polyhedral meshes

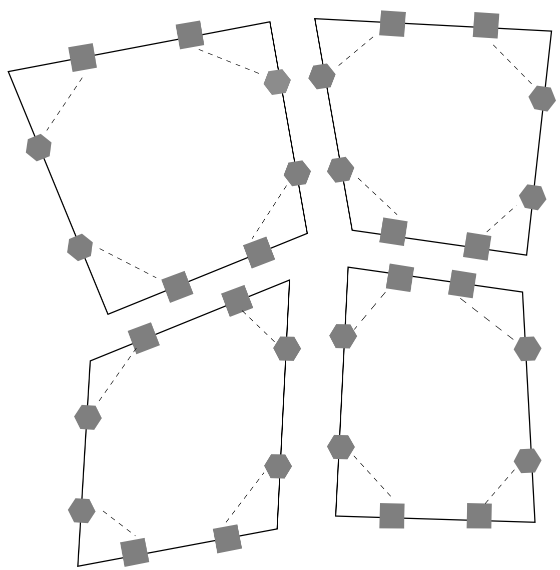


- 68% of interior mesh faces are non-planar



Recent and future developments

- use the family of MFD methods to attack other computational problems
- extensions to other PDEs
- local-flux MFD methods (with I. Yotov)



- Fluxes are connected in small groups around mesh vertices. Thus,

$$\boldsymbol{u}^h = \widetilde{\mathcal{GRAD}}\, \boldsymbol{p}^h$$

where $\widetilde{\mathcal{GRAD}}$ has a local stencil.

Conclusion

- For diffusion problems on unstructured polygonal and polyhedral meshes, we developed a *family of mimetic finite difference* methods with the following properties:
  - methods are computationally cheap
  - they have optimal convergence rates
  - and result in SPD matrices